Soviet electrochemistry 1987 vol.22 N8, pages 1054-1056

FREE ENERGIES OF ACTIVATION FOR THE REDUCTION OF AROMATIC NITRO COMPOUNDS.

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Abstract

Results are presented which were obtained when studying by the faradic-impedance technique the heterogeneous reaction of transfer of the first electron to molecules of a series of aromatic nitro compounds in dimethylformamide (DMF) at the mercury electrode, and are compared with the results iof E//s calculations of R. A. Marcus and Yu. I. Kharkats. The electrode impedance was measured at 20 degree C over the frequency range from 0. 12 to 20 kHz. A comparison of quantities DELTA G//I** does not equal and DELTA G//I//I** does not equal with the DELTA G//e//x** does not equal provides evidence in favor of an orientation of the electroactive molecules toward the electrode surface, over the concentration range studied, where the major semiaxis of the ellipsoid is perpendicular to the surface. As expected, the calculations which take into account the real geometry of the molecule yield results which are very close to the experimental ones.